CRD

Computational Research Division Report

Berkeley Lab

Office of Science
U.S. Department of Energy

APRIL 2007

# Clean Burning

## Combustion research seeks to quantify pollutant formation, lead to better turbine designs

Research to quantify the formation of pollutants during natural gas combustion has received 1.5 million computing hours from NASA. Led by Marc Day in CRD's Center for Computational Sciences and Engineering, the project, "Flame Dynamics and Emission Chemistry in High-Pressure Industrial Burners," was one of the four awarded by NASA last month under its National Leadership Computing System initiative.

The initiative sets out to support computationally intensive projects that advance a wide range of national interests, includes projects geared at improving aerospace vehicle design and climate change predictions.

Day will compute on the Columbia system (2,048-processor SGI Altix) at the NASA Advanced Supercomputing (NAS) facility, located at the Ames Research Center in Moffett Field, California.

"This is the second year now we've had the opportunity to access the Columbia computing resources," Day said. "In the first year, we created several terabytes of very interesting data, giving us and our experimental colleagues beautiful and complicated pictures of turbulent flame dynamics. This year, the calculations have stepped up another notch and now have a distinct practical purpose.

"The new project is an even greater challenge in terms of creating and then ingesting the huge simulation data sets, and developing new tools that help us to complete a picture of what's going on in these complex systems," he added.

Day and his fellow researchers plan to simulate natural gas combustion in

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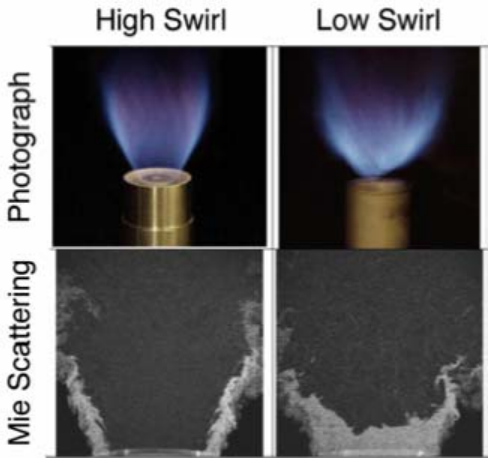


**The images show the turbulent high- and low-swirl atmospheric flames, as seen in the LBNL Combustion Lab. Time-averaged (photographs) and instantaneous (Mie scattering) images depict a complex interplay between combustion chemistry and aerodynamic flame stabilization, leading to extremely challenging computing requirements. Marc Day's project will explore such flames in an even more demanding high-pressure environment.**

# Cyber Digs

## Internet technology enables archaeologists to share and publish data

The Alexandria Archive Institute has enlisted Berkeley Lab's help in promoting the launch of an online tool for sharing and publishing primary archaeological data, a project that aims to make museum collections and field finds more accessible to scientists and students.

The institute, a nonprofit funded primarily by the William and Flora Hewlett Foundation, hopes to make Open Context the web tool archaeologists turn to not only for unearthing valuable information but also broadening the impact of their own research.

The institute's goal is not to run its own online archive, but to provide universities, museums or other organizations the software necessary for running an interactive database.

Eric Kansa, the institute's executive director, used Berkeley Lab's Access Grid in early April to demonstrate Open Context to attendants from six universi-

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# Heating Up

## Global warming will fuel more intense hurricanes

Michael Wehner's talk on hurricane research and scientific tools for making climate predictions was a big draw at NERSC earlier this month and coincided with the growing international interest in global warming and the human impact on climate change.

Wehner, CRD's resident climatologist, was a featured speaker at a brown-bag lunch series aimed at fostering a closer collaboration between NERSC staff and users. Past speakers included CRD astrophysicists Peter Nugent and Julian Borrill.

Launching his talk with a humorous quote by chaos theory pioneer Ed Lorenz, "Climate is what you expect … weather is what you get," Wehner outlined results from his recent work that showed a clear link between human activities and a rise of intense hurricanes.

Using 22 climate models that take into account natural and man-made forces, such as solar irradiance and black carbon aerosols, Wehner and his collaborators

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## Hall of Fame

### Taking ACTS On the Road

Osni Marques

Osni Marques of CRD's Scientific Computing Group gave one of four semi-plenary lectures at the International Conference on Computational Methods (ICCM 2007) in Hiroshima, Japan earlier this month.

In his talk, "Rewards of software reuse and an outlook on scientific software libraries," Marques described the functionalities currently available in the DOE Advanced Computational Software (ACTS) Collection, lessons that have been learned through an interaction with tool developers and users, the rewards of outreach efforts and hands-on activities, and scientific applications that have benefited from these tools.

The ACTS Collection is a set of DOE-developed software tools, sometimes in collaboration with other funding agencies, that make it easier to write high performance codes for engineering and computational science application codes. Marques and fellow CRD scientist Tony Drummond provide maintenance, outreach and training for the ACTS Collection of DOE-developed software tools.

The ICCM 2007 conference, which took place from April 4 to 6, provided an international forum for the presentation and showcase of recent advances in various aspects of computational methods. It reflected the state of the art of the computational methods involving theory, algorithm, programming, coding, numerical simulation, error and uncertainty analysis and/or the novel application of computational techniques to problems in engineering, science and other disciplines related to computations. Learn more about the conference at http://home.hiroshima-u.ac.jp/iccm2007.

### Parallel Programming

Kathy Yelick

Kathy Yelick, head of the Future Technologies Group in CRD, was the general chair of the ACM SIGPLAN 2007 Symposium on Principles and Practice of Parallel Programming (PPoPP), which took place in San Jose, California last month.

PPoPP provided a forum for papers and posters on the principles and foundations of parallel programming, tools and techniques for parallel programming and experiences in using parallel programming to solve applications problems.

This year's program includes two keynote addresses, 22 presentations, 18 posters and three tutorials. PPoPP was co-located with the 2007 International Symposium on Code Generation and Optimization (CGO).

Other CRD staff helped Yelick to make the program a success, including Costin Iancu and Parry Husbands. John Mellor-Crummey from Rice University was the program chair.

Check out slides of keynote presentations and other program information at http://ftg.lbl.gov/ppopp07.

### Math for Climate Study

The Mathematical Sciences Research Institute (MSRI) invited CRD scientists Phil Colella and Kathy Yelick to speak at a climate change symposium, "From Global Models to Local Action," this month in Berkeley, California.

The symposium featured climate experts from Europe, China and the United States. The goal was to engage the mathematical sciences community in addressing the issues involved in translating global, long-term predictions of climate change into local forecasts relevant for public and private sector policy.

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## Combustion *continued from page 1*

power-generation turbines in order to determine the mechanisms that modulate the production of pollutants, especially nitrogen oxides.

Nitrogen oxides contribute to the formation of acid rain, and can also cause serious respiratory problems. Understanding the mechanisms that produce nitrogen oxide in turbulent flames could lead to better designs of turbine combustors and ultimately to cleaner methods of producing electricity.

Simulation of these systems has the potential to provide a unique and critical role, since these high-pressure scenarios operate in an environment that is hostile to a wide range of traditional experimental diagnostics (problems include reduced optical access, laser field attenuation, signal quenching, pressure-induced flame thinning, etc).

The development of the simulation code, LMC, has been a key technology enabling Day's research into premixed burning. LMC implements a complex but highly efficient approach to advancing the equations of motion for a reacting gas in the special but very important regime, where convection is slow relative to the speed of acoustic waves.

Combining the large time steps afforded through these so-called low Mach number approaches with a dynamically adaptive grid scheme, LMC is uniquely capable of marshalling thousands of distributed memory processors to simulate turbulent combustion systems. It is the only tool presently able to do so at the spatial and temporal scales observable in laboratory experiments.

Day plans to carry out a number of studies to investigate the combined roles of injector swirl and fuel-air mixtures on pollutant production. Highly swirled injection, the baseline approach, results in a strong recirculation of heat that robustly stabilizes natural gas flames at the premixed fuel nozzle. But these recirculation zones dramatically increase the amount of time the exhaust stays in the heated chamber environment. Longer residence times in the heated exhaust streams lead to unacceptably high pollutant emissions.

Low-swirl injectors (LSI) are a new burner design developed by Robert

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# Archaeology *continued from page 1*

ties, including the University of Arizona, University of Arkansas and Pennsylvania State University.

"Archaeology is a good example of the challenges faced in many areas of 'small science.' Research programs are typically very case-specific, and there are few generally applied standards of recording. That makes meaningful data sharing and data integration very difficult," Kansa said. "With Open Context, we have tools to make data sharing easy and make it easy to browse, search, and query these results."

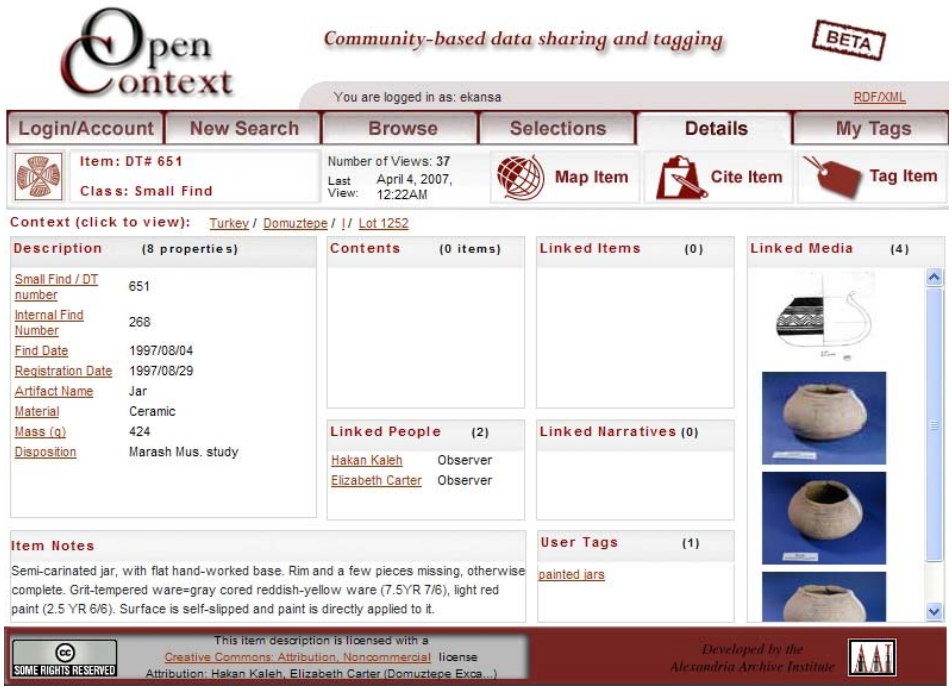
Kansa, who started the institute five years ago, makes a good advocate for using open source technologies in archaeology. While working on his Ph.D. in archaeology at Harvard University, he became frustrated at having to spend an inordinate amount of time tracking down information at the library that ultimately became endnotes and bibliographies.

He said the "tedious grind of tracking information down" prompted him to think about how file-sharing technologies can save time and cost for scientists and students. He is currently the organizer of the Society for American Archaeology's Digital Data Interest Group (DDIG), a body that now includes some 700 members.

Kansa founded the institute with his wife, Sara Whitcher Kansa, a zooarchaeologist who works on Domuztepe, a late Neolithic site in south central Turkey. Some of her field notes are used to demonstrate Open Context.

Kansa is one of a growing number of scientists who have become active proponents of open source technologies in archaeology, where researchers work in small teams with limited budgets. Yet, to answer key questions about human history, they need to examine a large amount of data—such as maps, drawings and vocal recordings—and put them in context.

"Conventional publication just isn't well suited for sharing the large and complex mass of multimedia documentation that archaeologists produce in even one project," Kansa said. "Conclusions get published much more than underlying data, and without the primary sources, it's hard to test the validity of those conclusions. Worse, without publication, primary documentation is very vulnerable to loss, and that represents an irreplaceable loss of world heritage."




**Open Context enables researchers and students in archaeology to contribute and search for primary field data. The site also provides opportunities for scientists to have their work cited more frequently.**

In recent years, government funding has become available for scientists to study the benefits of merging Internet technology with research. The National Science Foundation, for example, has funded an Arizona State University project to look at how cyberinfrastructure can provide archaeologists the access to large-scale data for comparing findings and answering broader questions about human history.

To develop Open Context, Kansa and his staff worked with David Schloen, an associate professor of archaeology at the University of Chicago and the head of a project called Online Cultural Heritage Research Environment (OCHRE). OCHRE is an expanding archaeological database from scientists including archaeologists, cultural anthropologists and linguists.

Integrating data that were documented in disparate ways and came in different media and languages (e.g., Egyptian hieroglyphs) is a formidable challenge.

Schloen has adapted XML, the common web markup language, to create ArchaeoML which makes it easy to store and search those field data. ArchaeoML forms the backbone of Open Context, which Kansa demonstrated over the Access Grid.

During his demonstration, Kansa showed how users could browse data from a particular archaeological site and organize the information through tagging. This way, the users can build up their own research files for future reference while making it easy for others to find them as well.

"Open Context lets a user community incrementally integrate results from different projects. It's really a learning system, and as it gets used, more meaningful linkages emerge across results from different projects."

Kansa plans to release the 1.0 version of Open Context and its source code within the year.

Check out Open Context at http://www.opencontext.org. Learn more about the Alexandria Archive Institute at http://www.alexandriaarchive.org.

# Global Warming

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concluded that humans have been responsible for the rise of sea surface temperature in hurricane-forming regions over the last century. Warm ocean water is a necessary ingredient for forming and strengthening hurricanes.

As a result of their research, the scientists calculated an 84-percent chance that human-related causes, especially the increase in greenhouse gases, led to at least 67 percent of the observed rise of sea surface temperatures. The warming trend not only led to an increase in the number of hurricanes overall, but more intense ones as well (category 4 and 5 hurricanes).

The trend will continue, Wehner said. Already, his research is predicting that by 2020, the rise of sea surface temperatures in the Atlantic hurricane-forming region will double the warming that occurred throughout the entire 20th century.

"You can see humans are causing this change in more intense hurricanes," Wehner said.

The exhaustive work, which involved scientists from Lawrence Livermore National Lab, the National Center for Atmospheric Research and others, was published in the Proceedings of the National Academy of Sciences on Sept. 12, 2006.

Wehner's talk was particularly timely given an increasing interest by the U.S. and other countries to assess humans' contribution to global warming and its negative impact on the environment. The Intergovernmental Panel on Climate Change just released the second of a four-part report detailing the effects of climate change on different regions of the world.

Wehner noted that computer modeling of historical data is key to predicting climate change, given that scientists don't have a way to conduct controlled experiments on a different planet. He would like to see more U.S. computing resources devoted to climate simulations, as well as more efforts to develop better climate models.

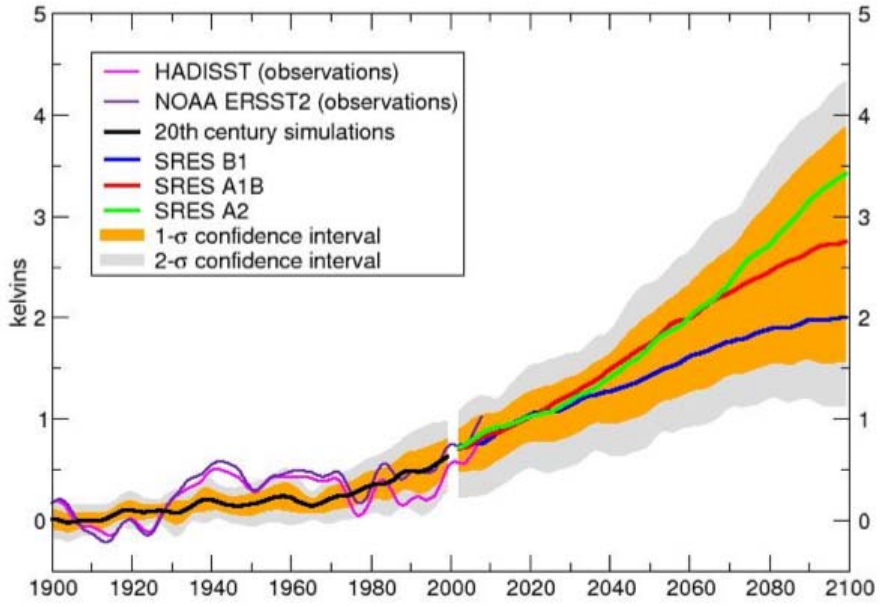
In fact, Wehner was the lead author in a paper that looked at how petascale computing can improve climate modeling by including better calculations of atmospheric variables such as clouds. Achieving high-resolution simulations on the kilometer scale, however, would require a 10-petaflop/s computer, Wehner said. The paper, co-authored by CRD's Lenny Oliker and NERSC's John Shalf, will be published in the next issue of the International Journal of High Performance Computing Applications.

"Simulations offer our only hope in predicting the climate change. I think NERSC is in the right place to do this," Wehner said.

Currently, Wehner is focused on projects that take a closer look at how certain climate variables, such as moisture in the atmosphere and wind, affect hurricane formation.

Read the PNAS article at http://www.pnas.org/cgi/reprint/0602861103v1.

## 21st Century Ocean Temperature Changes in the Atlantic Hurricane Formation Area




Warm ocean waters fuel hurricanes, and this image depicts a three-day average of actual sea surface temperatures (SSTs) for the Caribbean Sea and the Atlantic Ocean from August 25-27, 2005. Every area in yellow, orange or red represents 82 degrees Fahrenheit or above. A hurricane needs SSTs at 82 degrees or warmer to strengthen. The data came from the Advanced Microwave Scanning Radiometer (AMSR-E) instrument on NASA's Aqua satellite. Image courtesy of NASA/SVS.

## Combustion *continued from page 1*

Cheng in LBNL's Environmental Energy Technologies Division. LSI devices are carefully designed to stabilize premixed flames aerodynamically without creating a large recirculation zone. Cheng has put his concept to test in a prototypical industrial furnace as a drop-in replacement to the "SoLoNOx" commercial turbine injector configuration. And while the burner has performed admirably, the high-pressure rig allows only a limited set of diagnostics, and prevents collection of sufficiently detailed data necessary for further refinements in the designs of the low-swirl injector device.

Day's proposed simulations will provide unprecedented detail about the flame stability and emissions characteristics of this class of swirl burners. However, the real hope is that the mountains of data will help to shed light on the fundamental processes responsible for pollutant formation, how these processes are affected by pressure and turbulence and, in turn, how the flame and turbulence can be controlled to optimize the overall performance. Modern combustion research has made a significant impact in the reduction of pollutants produced by industrial combustion applications. Over the last three decades, nitrogen oxide emission standards have been successfully reduced to less than 25 ppm, due in a large part to the implementation of advanced combustion concepts. Cheng's low swirl technology has the potential to further reduce these levels to an astounding 5 ppm. Given the degree to which U.S. industry remains invested in combustion-based energy technology, understanding and optimizing the performance of these ultra-low pollution combustion devices will go a long way towards protecting the global environment.

For more information on Day's work in CRD, visit the CCSE web page at http://seesar.lbl.gov/ccse. Check out http://eetd.lbl.gov to learn more about LBNL's work on energy technologies. The NASA Advanced Supercomputing Division has featured Day's work on its web site, http://www.nas.nasa.gov.

## Hall of Fame

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Colella, head of the Applied Numerical Algorithms Group in CRD, gave a talk titled "Algorithms for the Study of Climate Change." Yelick, head of the Future Technologies Group, presented "Architectural Trends and Programming Model Strategies for Large-Scale Machines."

Another Berkeley Lab scientist, Bill Collins, also spoke at the conference. Collins, who joined the lab's Earth Sciences Division recently, came from the National Center for Atmospheric Research (NCAR) in Colorado. He was a lead author of the Intergovernmental Panel on Climate Change's 2007 report.

The symposium addressed several major challenges in climate projection, including the formulation of climate models, the construction of risk analyses for climate impacts and the extraction of climate information for decision-making.

### Nuclear Simulations

Phil Colella

The 2007 Computational Science and Engineering Conference (CESC2007) in Washington, D.C. earlier this month featured Phil Colella as one of its speakers. Colella, head of CRD's Applied Numerical Algorithms Group, gave the talk "Structured-Grid Adaptive Methods for Partial Differential Equations in Complex Geometries."

The conference brought together scientists to discuss technical and policy issues in high-performance computing. This year, the conference focused on nuclear energy and reactor simulations.

The conference also included government officials, such as Peter B. Lyons from the U.S. Nuclear Regulatory Commission, Christopher King from the House Committee of Science and Technology and Kathryn Clay from the Senate Committee on Energy and Natural Resources.

### Power and Petascale

Horst Simon

Horst Simon, Associate Lab Director of Computing Sciences and head of CRD, gave a keynote speech titled "Parallelism and Power in the Age of Petascale Computing" at the IEEE International Parallel and Distributed Processing Symposium last month.

The talk explored the challenges of dealing with increasing parallelism and reducing power consumption as the computing community moves toward petascale computing. Aside from explaining how these two issues are interrelated, Simon also pointed out that low-power solutions are not necessarily the most energy-efficient solutions.

Simon ended his talk by outlining a multi-tier strategy for solving the power issue. He advocated attacking the problem at the component, system, computer room and building environment level. John Shalf, who leads the Science-Driven System Architecture Team at NERSC, co-authored the report.

His talk opened the workshop on high-performance, power aware computing at the symposium. Learn more about the workshop at http://hppac.cs.vt.edu.

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# Exascale Computing

Michael Strayer (upper left), Associate Director for Advanced Scientific Computing Research (ASCR) at the DOE Office of Science, addressed the gathered scientists at a two-day meeting.

Nearly 150 researchers from national labs and universities attended a two-day "town hall meeting" on the proposed Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security (E3SGS) program. The goal of the meeting, along with subsequent gatherings scheduled for May 17-18 at Oak Ridge and May 31-June 1 at Argonne, is to come up with an innovative program of novel computational science challenges to expand the contributions of ASCR programs to the DOE Office of Science mission over the next decade.

ASCR Associate Director Michael Strayer told the assembled participants that he was looking to them to help "set the vision and the standard of where we could be as we evolve over the next 10 years." The scientists broke into nine groups and discussed topics such as renewable energy, computational biology and parallel computing. Results from these groups will be further refined at the Oak Ridge and Argonne meetings.

Berkeley Lab Director Steve Chu addressed town hall meeting participants on the second day, giving a lunch-hour presentation on LBNL's increasing emphasis on energy efficiency and new, renewable energy sources. Chu underscored his case for increased investment by citing both economic and environmental factors, which show that current energy practices are too costly to sustain on a global scale.

More information about E3SGS and reports from the breakout groups can be found at http://hpcrd.lbl.gov/E3SGS/main.html.

## Hall of Fame

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### Student Program

Juan Meza

Juan Meza, head of the High Performance Computing Research Department, along with two graduate assistants will lead 12 students in math research projects as part of the 2007 Mathematical Sciences Research Institute Undergraduate Program (MSRI-UP).

The program seeks to increase the number of undergraduate students from underrepresented groups in mathematics graduate programs. MSRI-UP includes summer research opportunities, mentoring, workshops on the graduate school application process and follow-up support.

## About CRD Report

CRD Report, which publishes every other month, highlights the cutting-edge research conducted by staff scientists in areas including turbulent combustion, nano materials, climate change, distributed computing, high-speed networks, astrophysics, biological data management and visualization. CRD Report Editor Ucilia Wang can be reached at 510 495-2402 or Uwang@lbl.gov. Find previous CRD Report articles at http://crd.lbl.gov/html/news/CRDreport.html.